

# On the Crystallinity of Silicate Dust in the Interstellar Medium

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## ABSTRACT

An accurate knowledge of the mineralogy (chemical composition and crystal structure) of the silicate dust in the interstellar medium (ISM) is crucial for understanding its origin in evolved stars, the physical and chemical processing in the ISM, and its subsequent incorporation into protostellar nebulae, protoplanetary disks and cometary nuclei where it is subjected to further processing. While an appreciable fraction of silicate dust in evolved stars, in protoplanetary disks around pre-main sequence stars, in debris disks around main sequence stars, and in cometary nuclei is found to be in crystalline form, very recent infrared spectroscopic studies of the dust along the sightline toward the Galactic center source Sgr A\* placed an upper limit of  $\sim 1.1\%$  on the silicate crystalline fraction, well below the previous estimates of  $\sim 5\%$  or  $\sim 60\%$  derived from the observed  $10\ \mu\text{m}$  absorption profile for the local ISM toward Cyg OB2 No.12. Since the sightline toward Sgr A\* contains molecular cloud materials as revealed by the detection of the  $3.1$  and  $6.0\ \mu\text{m}$  water ice absorption features, we argue that by taking into account the presence of ice mantles on silicate cores, the upper limit on the degree of silicate crystallinity in the ISM is increased to  $\sim 3\text{--}5\%$ .

**Key words:** ISM: dust, extinction – Galaxy: center – infrared: ISM: line and bands – ISM: diffuse ISM, molecular clouds

## 1 INTRODUCTION

The mineralogical composition of dust contains important information about its origin and evolution, and may reveal the physical, chemical and evolutionary properties of the astrophysical regions where the dust is found. Silicate, one of the major components of cosmic dust species, is ubiquitously seen in various astrophysical environments, ranging from the Galactic diffuse interstellar medium (ISM), HII regions, and the dust torus around active galactic nuclei to dust envelopes around evolved stars, protoplanetary disks around pre-main sequence stars, debris disks around main sequence stars, cometary comae and interplanetary space. Their chemical composition and crystal structure vary with local environments.

Interstellar spectroscopy provides the most diagnostic information on dust composition. In the infrared (IR), the strongest interstellar spectral features are the  $9.7$  and  $18\ \mu\text{m}$  absorption (or emission) bands which are generally attributed to the Si–O stretching and O–Si–O bending modes, respectively. While the absorption profiles measured in laboratory for crystalline olivine and pyroxene show many sharp

features, in the diffuse ISM, the observed  $9.7$  and  $18\ \mu\text{m}$  silicate features are broad and relatively featureless, suggesting that interstellar silicates are mainly amorphous rather than crystalline. Since the crystallinity of silicate dust is intimately connected to the energetic processing occurred in the evolutionary life cycle of dust and depends on the environmental properties, of particular interest to silicate astromineralogy is the abundance of crystalline silicates in different astrophysical environments, especially in the diffuse ISM.

Recently, a number of studies have been made to determine the crystallinity degree of silicates in the diffuse ISM. From the observed  $9.7\ \mu\text{m}$  absorption profile for dust in the local ISM toward Cyg OB2 No.12, Li & Draine (2001) estimated the fraction of Si in crystalline silicates to be  $\leq 5\%$ . Demyk et al. (1999) derived an upper limit of  $\sim 1\text{--}2\%$  of crystalline silicates in mass toward two massive protostars. However, Bowey & Adamson (2002) argued that a complex mixture of crystalline silicates (60% by mass) and amorphous silicates (40% by mass) could explain the observed smooth silicate absorption profile at  $9.7\ \mu\text{m}$  toward Cyg OB2 No.12. More recently, Kemper, Vriend & Tielens (2004) placed a more strict constraint of  $\leq 1.1\%$  on the crystallinity of interstellar silicates, based on a detailed analysis of the  $9.7\ \mu\text{m}$  feature obtained with the Short Wavelength

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Spectrometer (SWS) on board the Infrared Space Observatory (ISO). This upper limit  $\sim 1.1\%$  of crystalline silicates was derived from a direct comparison of the Sgr A\* spectrum with theoretical spectra for pure silicates.

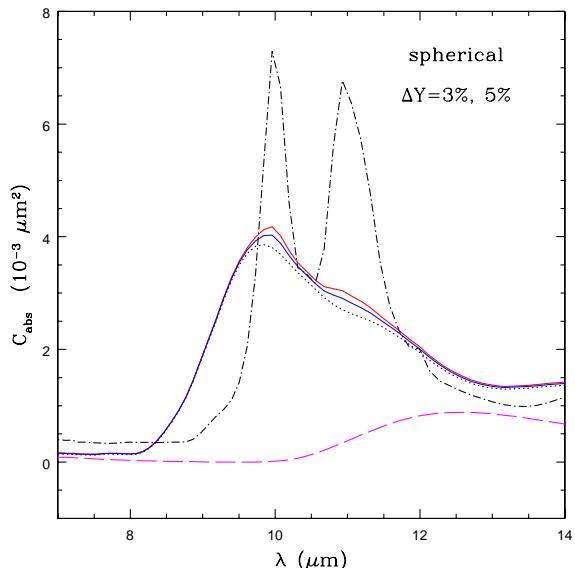
However, it is evident from the detection of the 3.1 and 6.0  $\mu\text{m}$  water ice features respectively attributed to the O–H stretching and bending modes that there are molecular cloud materials along the line of sight toward Sgr A\* (McFadzean et al. 1989; Tielens et al. 1996; Chiar et al. 2000). This is further confirmed by the detection of solid CO<sub>2</sub> absorption toward Sgr A\* (Lutz et al. 1996; de Graauw et al. 1996). In order to infer the precise mineralogical composition of dust, we have to take the grain ice mantles into account when interpreting the observed silicate features. Indeed, in this paper we show that ignoring the ice mantles coated on the silicate cores can result in an underestimation of the crystalline degree of silicate dust, as much as  $\sim 3\text{--}5\%$ .

The purpose of this work is to address the question how the ice mantles affect the determination of dust mineralogical composition (i.e. whether and to what degree the inclusion of ice mantles will hide the sharp features of crystalline silicates and lead to an underestimation of the silicate crystallinity), not to model any specific astronomical objects. Therefore, neither the specific choice of silicate dielectric functions nor the precise constituents of the ice mantles would affect our conclusion.

## 2 VOLUME FRACTION OF WATER ICE

The sightline toward the Galactic center source Sgr A\* suffers about  $\sim 30$  mag of visual extinction (e.g. see McFadzean et al. 1989), to which molecular clouds may contribute as much as  $\sim 10$  mag (Whittet et al. 1997). Except for H<sub>2</sub>O features, there are many additional molecular absorption features, attributed to CO<sub>2</sub>, NH<sub>3</sub>, CO, CH<sub>3</sub>OH, CH<sub>4</sub> and other species. These icy molecules might accrete on the pre-existing silicate core inside dense molecular clouds and form an ice mantle. As for further evolution, the accreted icy grain mantles could be photoprocessed and converted into organic refractory residues (Greenberg et al. 1995).

Assuming the 3.1  $\mu\text{m}$  water ice absorption results from the water ice mantles uniformly coated on silicate grains which produce the 9.7  $\mu\text{m}$  absorption, we estimate the volume ratio of the ice mantles to the silicate cores from the observed optical depths –  $\tau_{3.1}$  for the 3.1  $\mu\text{m}$  O–H feature, and  $\tau_{9.7}$  for the 9.7  $\mu\text{m}$  Si–O feature. Let  $V_{\text{sil}}$  and  $V_{\text{ice}}$  respectively be the volumes of the silicate cores and the ice mantles. Let  $A_{\text{ice}}^{3.1}$  and  $A_{\text{sil}}^{9.7}$  be the integrated band strength for the 3.1  $\mu\text{m}$  O–H feature and the 9.7  $\mu\text{m}$  Si–O feature, respectively. For spherical silicate core–ice mantle grains, we use Mie theory (Bohren & Huffman 1983) to obtain  $A_{\text{ice}}^{3.1} = \int_{3.1 \mu\text{m}} (C_{\text{ice}}^{3.1}/V) d\lambda$  and  $A_{\text{sil}}^{9.7} = \int_{9.7 \mu\text{m}} (C_{\text{sil}}^{9.7}/V) d\lambda$ , where  $C_{\text{ice}}^{3.1}$  ( $C_{\text{sil}}^{9.7}$ ) is the continuum-subtracted absorption cross section of the 3.1  $\mu\text{m}$  (9.7  $\mu\text{m}$ ) ice (silicate) feature, and  $V$  is the volume of a spherical grain with radius  $a$ . For the Sgr A\* sightline,  $\tau_{3.1} \approx 0.50$  and  $\tau_{9.7} \approx 3.52$  (Chiar et al. 2000). We therefore obtain  $V_{\text{ice}}/V_{\text{sil}} = (\tau_{3.1}/\tau_{9.7}) (A_{\text{sil}}^{9.7}/A_{\text{ice}}^{3.1}) \approx 0.55$ ,



**Figure 1.** Absorption cross sections of spherical grains for  $V_{\text{ice}}/V_{\text{sil}} = 0.55$ . Dotted: amorphous silicate core–ice mantle grains ( $C_{\text{abs}}^{\text{am}}$ ); dot-dashed: crystalline olivine silicate core–ice mantle grains ( $C_{\text{abs}}^{\text{crys}}$ ); long-dashed: equal-volume ice spheres for the ice mantles; solid:  $C_{\text{abs}} = C_{\text{abs}}^{\text{am}} + \Delta Y C_{\text{abs}}^{\text{crys}}$  where  $\Delta Y = 5\%$  is the crystalline olivine silicate fraction; short-dashed:  $C_{\text{abs}} = C_{\text{abs}}^{\text{am}} + \Delta Y C_{\text{abs}}^{\text{crys}}$  with  $\Delta Y = 3\%$ . Note that water ice produces a shoulder at  $\lambda > 11 \mu\text{m}$ . This should not be interpreted as a crystalline silicate feature.

assuming that all silicate grains are coated by a layer of ice mantle.<sup>1</sup>

## 3 SPHERICAL GRAINS

We consider 3 types of dust materials: amorphous olivine, crystalline olivine, and pure water ice. We adopt the dielectric functions of Dorschner et al. (1995) for amorphous olivine, of Li & Draine (2001) for crystalline olivine, and of Hudgins et al. (1993) for water ice.

We first consider spherical silicate core–water ice mantle grains. We take the silicate core size to be  $a_{\text{sil}} = 0.1 \mu\text{m}$ , a typical size for interstellar dust. We should note that the choice of an exact grain size is not critical since in the wavelength range considered here submicron-sized interstellar grains are in the Rayleigh regime. Also because of this, we do not need to consider dust size distributions.

In Figure 1 we plot the absorption cross sections for amorphous olivine silicate core–H<sub>2</sub>O ice mantle grains and for crystalline olivine silicate core–H<sub>2</sub>O ice mantle grains. As shown in Figure 1, the absence of narrow features near 10.0 and 11.1  $\mu\text{m}$  in the absorption spectrum suggests that

<sup>1</sup> In reality, a thicker ice mantle would be expected for the silicate dust in the molecular cloud component which contributes about 10 mag to the total  $\sim 30$  mag of visual extinction toward Sgr A\*. An ice mantle as thick as  $V_{\text{ice}}/V_{\text{sil}} \approx 7.6$  was implied for the dust in the dense molecular cloud toward the field star Taurus Elias 16 (Bowey et al. 1998). A thicker ice mantle would hide up a larger fraction of crystalline silicates.

the inclusion of water ice mantles would hide up  $\sim 3\text{--}5\%$  crystalline mass fraction without being noticed. Note that water ice has a broad absorption band at  $\sim 12.2\text{ }\mu\text{m}$  (see Fig. 1; Léger et al. 1983; Hudgins et al. 1993). The inclusion of an ice mantle on silicate dust (no matter it is amorphous silicate or crystalline silicate) results in a weak shoulder at  $\lambda > 11\text{ }\mu\text{m}$ . This is noticeable even in the model spectrum of ice-coated pure amorphous silicate dust (see Fig. 1). One should caution that this should not be interpreted as a crystalline silicate feature.

We also consider a model in which only the molecular cloud dust is coated with a layer of ice mantle. If we assume that silicate dust and carbon dust equally contribute to the  $\sim 10$  mag visual extinction, the volume ratio of the ice mantle to the silicate core for the molecular cloud dust would be  $V_{\text{ice}}/V_{\text{sil}} \approx 0.83$ . The bare diffuse cloud dust is responsible for the remaining  $\sim 20$  mag visual extinction. In Figure 2 we show the model cross sections obtained by summing up  $1/3$  of that produced by the molecular cloud dust and  $2/3$  of that produced by the diffuse cloud dust. Similarly,  $\sim 3\text{--}5\%$  crystalline silicate would be hidden because of the presence of an ice mantle on the molecular cloud dust toward Sgr A\*.<sup>2</sup>

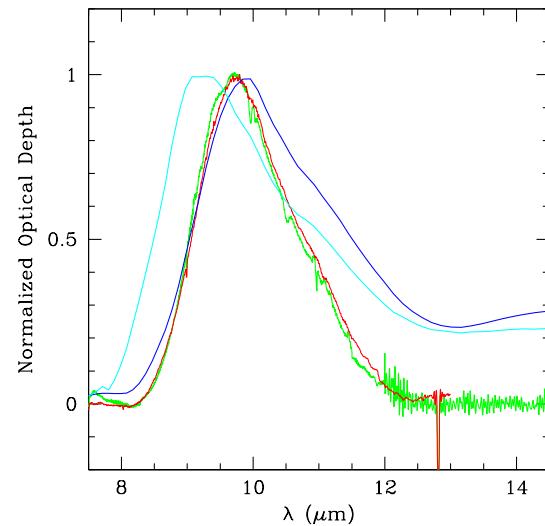
So far, we have only considered olivine silicate dust. It is possible that there is a considerable amount of pyroxene dust in the ISM (see Bowey & Adamson 2002 and references therein). For illustration, we carry out similar calculations for pyroxene and obtain similar conclusions (see Fig. 2). Again, we should stress that the purpose of this work is not to model any specific astronomical objects, but to investigate the effects of ice mantles on the silicate crystallinity estimation. We do not expect either olivine or pyroxene alone could closely reproduce the interstellar silicate absorption feature observed toward Sgr A\*. For comparison, we also show in Figure 2 the ISO spectra of Sgr A\* obtained by Kemper et al. (2004) and Gibb et al. (2004).<sup>3</sup> The fact that, while the  $10\text{ }\mu\text{m}$  feature of olivine peaks at relatively longer wavelengths than the observed spectra, pyroxene peaks at too short wavelengths, suggests the co-existence of both olivine and pyroxene in the ISM.

#### 4 SPHEROIDAL GRAINS

However, interstellar grains must be nonspherical as indicated by interstellar polarization. We now consider

<sup>2</sup> Admittedly, the approach adopted here is simplified. The molecular cloud silicate dust may differ from that of the diffuse cloud (e.g. their  $10\text{ }\mu\text{m}$  Si-O features may have different line profiles [particularly line widths], see Bowey, Adamson, & Whittet 2001 and references therein). Their optical properties which are temperature-dependent (Bowey et al. 2001) may also differ from each other since the molecular cloud dust is generally colder than the diffuse cloud dust (e.g. see Greenberg & Li 1996a). Moreover, it is not clear if the molecular cloud silicate dust has the same iron fraction as the diffuse cloud silicate dust (it is well recognized that, as most recently experimentally demonstrated by Bowey et al. [2007], the optical properties of silicate dust are very sensitive to the proportion of iron).

<sup>3</sup> We note that the ISO spectrum of Sgr A\* appears to have a feature at  $\sim 6.9\text{ }\mu\text{m}$ , attributed to crystalline melilite (Bowey & Hofmeister 2005).



**Figure 2.** Comparison of the ISO spectra of Sgr A\* (thick solid: Gibb et al. 2004; thick dashed: Kemper et al. 2004) and the absorption spectra of olivine (thin solid) and pyroxene (dot-long dashed) spheres with 3% crystallinity, with  $1/3$  of the dust coated by a layer of ice mantle ( $V_{\text{ice}}/V_{\text{sil}} = 0.83$ ) and  $2/3$  of the dust being bare silicates. The  $\lambda > 11\text{ }\mu\text{m}$  shoulder of the model spectra arises from the ice mantles (also see Fig. 1). Also shown is the absorption spectrum of pure amorphous olivine dust without an ice mantle (dot-short dashed).

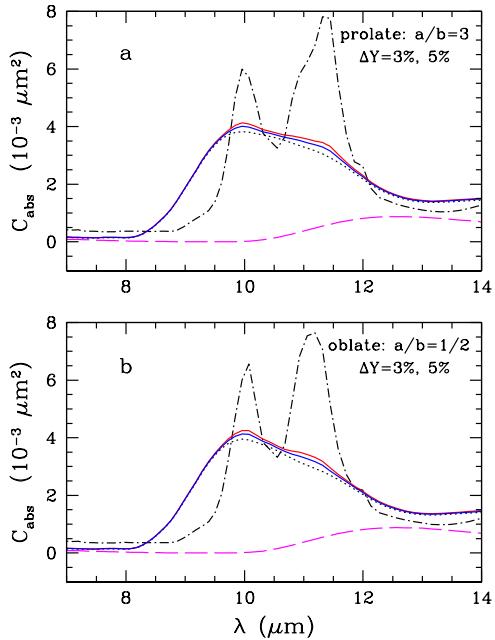
spheroidal shape which can be exactly solved in the Rayleigh limit (see Li et al. 2002 and references therein).

We consider confocal silicate core-ice mantle spheroidal grains with a volume-equivalent sphere radius  $r_{\text{sil}}^{\text{eq}} = (ab^2)^{1/3} = 0.1\text{ }\mu\text{m}$ , where  $a$  and  $b$  are the semi-axis along and perpendicular to the symmetry axis, respectively. Again, we take the volume ratio of the ice mantles to the silicate cores to be  $V_{\text{ice}}/V_{\text{sil}} = 0.55$ .

We first consider prolate grains with  $r_{\text{sil}}^{\text{eq}} = 0.1\text{ }\mu\text{m}$  for the silicate cores and  $a/b = 3$  for the ice mantles.<sup>4</sup> In Figure 3a we plot the absorption cross sections for ice coated-amorphous silicate prolates and ice coated-crystalline prolates. Just like spherical grains, the inclusion of water ice mantles would hide up  $\sim 3\%$  crystalline mass fraction without being noticed. Similarly, we perform the same calculations but for oblate grains with  $a/b = 1/2$  for ice mantles.<sup>5</sup> As seen in Figure 3b, a crystallinity degree of as much as  $\sim 3\%$  can be covered by the ice mantles.

<sup>4</sup> Greenberg & Li (1996b) found that prolates of  $a/b = 3$  provide an almost perfect match to the  $10, 18\text{ }\mu\text{m}$  silicate polarization features of the Becklin-Neugebauer (BN) object.

<sup>5</sup> Lee & Draine (1985) and Hildebrand & Dragovan (1995) found that  $a/b = 1/2$  oblates fit well the  $3.1\text{ }\mu\text{m}$  ice polarization and the  $10\text{ }\mu\text{m}$  silicate polarization of the BN object.



**Figure 3.** Same as Figure 1 but for (a)  $a/b = 3$  prolates and (b)  $a/b = 1/2$  oblates.

## 5 GRAINS WITH DISTRIBUTIONS OF ELLIPSOIDAL SHAPES

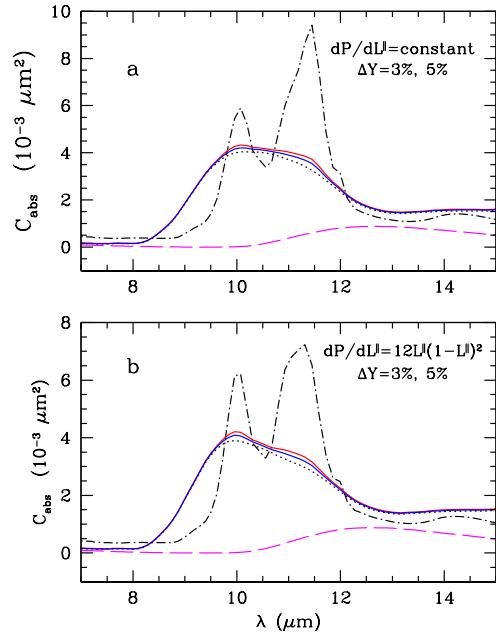
The shape of a spheroidal grain is characterized by its eccentricity  $e$  (and the depolarization factors  $L^{\parallel}$ ,  $L^{\perp}$  via eq.[4] of Li et al. 2002). In §4 we consider grains with a single shape. We now consider an average of a distribution of shapes. We assume two kinds of shape distribution functions: 1)  $dP/dL^{\parallel} = \text{constant}$ , i.e., all shapes are equally probable (Bohren & Huffman 1983); 2)  $dP/dL^{\parallel} = 12L^{\parallel}[1 - L^{\parallel}]^2$  (Ossenkopf, Henning, & Mathis 1992).<sup>6</sup>

Averaging over the shape distribution, we have the resultant absorption cross section  $C_{\text{abs}} = \int_0^1 dL^{\parallel} dP/dL^{\parallel} C_{\text{abs}}(L^{\parallel})$ , where  $C_{\text{abs}}(L^{\parallel})$  is the absorption cross section of a particular shape  $L^{\parallel}$  (note  $L^{\parallel}$  is for the mantle; the core depolarization factor is derived from eqs.[4-6] of Li et al. 2002). Again, we assume confocal geometry for core-mantle grains, with the above  $dP/dL^{\parallel}$  (as well as  $e$ ) applying to the outer surface.

The results are shown in Figure 4. Similar to spherical grains and grains of a single ellipsoidal shape, with  $\sim 3\%$  crystalline silicates included, the absorption profiles still do not seem to exhibit the sharp features of crystalline silicates.

## 6 SUMMARY

We have investigated the effects of ice mantles coated on silicate cores of various shapes on the determination of the crys-



**Figure 4.** Same as Figure 1 but (a) for grains with a uniform distribution of ellipsoidal shapes (i.e.  $dP/dL^{\parallel} = \text{constant}$ ) and (b) for grains with  $dP/dL^{\parallel} = 12L^{\parallel}[1 - L^{\parallel}]^2$ .

tallinity degree of silicates. It is found that for the dust in the line of sight toward the Galactic center source Sgr A\*,  $\sim 3\%$  crystalline silicates could be hidden by ice mantles, well exceeding the upper limit  $\sim 1.1\%$  of Kemper et al. (2004) derived from the assumption of the absence of dense molecular materials in this line of sight. We take the standard approach by assuming that the silicates are amorphous and then adding in crystalline components. But as shown in Kemper et al. (2004), the smooth, featureless  $10\text{ }\mu\text{m}$  amorphous silicate spectrum allows as much as  $\sim 2.2\%$  crystalline silicates (or even higher; see Bowey & Adamson 2002). Therefore, the total allowable degree of crystallinity would be  $\sim 5\%$ , consistent with the earlier estimates of Li & Draine (2001).

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<sup>6</sup> This distribution peaks at spheres ( $L^{\parallel} = L^{\perp} = 1/3$ ) and is symmetric about spheres with respect to eccentricity  $e$ . It drops to zero for the extreme cases: for infinitely thin needles ( $a \gg b$ )  $L^{\parallel} \rightarrow 0$ ; for infinitely flattened pancakes ( $a \ll b$ )  $L^{\parallel} \rightarrow 1$ .

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